

Pair condensation in a Finite Trapped Fermi Gas

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We study signatures of the superfluid phase transition and the pseudogap phase in a trapped finite-size system of spin-1/2 fermions with infinite scattering length. Applying the auxiliary-field quantum Monte Carlo (AFMC) method in the canonical ensemble, we compute the energy-staggering pairing gap, heat capacity, and condensate fraction as a function of temperature. Our calculations reveal clear signatures of the superfluid phase transition in all three quantities, including a signature of the lambda peak in the heat capacity. Comparing the temperature dependence of these quantities shows that the pairing gap does not exhibit an obvious pseudogap effect in this system.

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Cold atomic Fermi gases are an important paradigm in the study of strongly interacting quantum systems and of superfluidity. They provide clean and experimentally tunable strongly interacting systems that can be used as testbeds for the development of many-body methods, and their study can provide insight into the behavior of such diverse systems as neutron matter, quark matter and high-temperature superconductors [1–5]. They have been widely investigated experimentally, and many of their properties, such as thermodynamic functions, density profiles and spectral functions, have been measured [4, 6].

A key goal in the study of cold atomic Fermi gases is to accurately describe the superfluid phase transition in the unitary gas and, in particular, to understand to what extent pairing persists in the normal phase above T_c . In cold atomic Fermi gases, Bardeen-Cooper-Schrieffer (BCS) superfluidity is continuously connected to Bose-Einstein condensation (BEC) through a strongly-interacting crossover regime. This connection is enabled through s -wave scattering length a , which completely characterizes a zero-range interaction. In the BCS regime, where a is small and negative, pairing and superfluidity occur simultaneously at a critical temperature T_c . In the BEC regime, where a is small and positive, pairing occurs prior to condensation at a temperature $T^* \gg T_c$ owing to the existence of a deep two-body bound state; in this regime a nonzero gap exists above T_c . In the crossover regime, however, the effects of pairing are not completely understood.

Pairing is widely believed to occur above T_c in the crossover regime, and in particular in the unitary limit of infinite scattering length, giving rise to a so-called “pseudogap” phase (see Ref. [1] for an introduction). But the experimental characterization of this phase is incomplete. New radiofrequency spectroscopy techniques have provided evidence for pairing at and possibly above T_c by observing back-bending in the dispersion relation [7–10] (there is some ambiguity for $T > T_c$ because of the presence of a universal $1/k^4$ tail [11] in the momentum distribution). However, experiments have not yet determined the complete temperature dependence of the pairing gap

across the phase transition, which could provide one of the key signatures of the phase. Recently the heat capacity and compressibility were measured across the phase transition [12]; surprisingly, these quantities displayed no obvious signatures of a pseudogap above T_c , a result consistent with measurements of the equation of state for the pressure from another set of experiments [13–15].

Numerous Monte Carlo studies have been performed to study cold atomic Fermi gases. However, only a few [14, 17–19] have attempted to address the existence of a pseudogap phase above the superfluidity critical temperature. Even fewer have considered the thermodynamics of the trapped gas [20] or of finite-size systems.

Here we study signatures of the superfluid phase transition in the trapped, two-species (“spin-up” and “spin-down”), finite-size Fermi gas in the unitary limit of infinite scattering length. We apply the auxiliary-field Monte Carlo (AFMC) method in the canonical ensemble (of fixed number of spin-up and spin-down atoms) to accurately calculate the pairing gap, condensate fraction, and heat capacity as a function of temperature. We define the pairing gap as one-half the energy required to break a pair, $\Delta_{\text{gap}} \equiv [2E(N_{\uparrow}, N_{\downarrow} - 1) - E(N_{\uparrow}, N_{\downarrow}) - E(N_{\uparrow} - 1, N_{\downarrow})]/2$, where $E(N_{\uparrow}, N_{\downarrow})$ is the energy of the system with N_{\uparrow} spin-up and N_{\downarrow} spin-down atoms [6]. This is a model-independent quantity. Our calculations provide the first *ab initio* results for the temperature dependence of these quantities in a finite, trapped atomic system, and the first *ab initio* calculations for the energy-staggering pairing gap and heat capacity across the superfluid phase transition in any system of cold atoms. Our results are particularly relevant in light of recent advances in experiments with finite-size quantum gases [21].

Hamiltonian and model space.—We consider equal numbers $N_{\uparrow} = N_{\downarrow} = N/2 = 10$ of two species of fermions interacting at very short range in a spherical harmonic trap with frequency ω . The interaction $V(\mathbf{r})$ is modeled as a contact interaction $V(\mathbf{r}) = V_0\delta(\mathbf{r})$, which acts only in the s -wave channel and therefore allows only particles of different species to interact. We apply the AFMC method in the framework of a configuration-interaction (CI) shell model space spanned by the single-particle

eigenstates $|nlm\rangle$ of the harmonic trap (n is the radial quantum number, l is the orbital angular momentum and m is its projection) with energies $\varepsilon_{nl} = (2n + l + 3/2)\hbar\omega$. The model space is truncated to \mathcal{N}_{\max} oscillator shells, i.e., we take only oscillator states with $2n + l \leq \mathcal{N}_{\max}$. We denote the total number of such states by \mathcal{N}_s . By studying the convergence of observables as a function of \mathcal{N}_{\max} we determine a cutoff for which the observables are well-converged at all temperatures of interest. The interaction strength V_0 for each value of \mathcal{N}_{\max} is tuned to reproduce the exact ground state energy E_0 of the two-particle system ($E_0 = 2\hbar\omega$ at unitarity).

AFMC method.—The AFMC method works by applying a Hubbard-Stratonovich (HS) transformation [22] to the propagator $e^{-\beta\hat{H}}$ (where β is the inverse temperature T) and evaluating the resulting multidimensional path integral by Monte Carlo methods. We apply the CI shell model formalism commonly used in nuclear physics [23–26]. The thermal propagator is expressed as a path integral

$$e^{-\beta\hat{H}} \approx \int D[\sigma] G_\sigma \hat{U}_\sigma, \quad (1)$$

where the integration is over auxiliary fields $\sigma(\tau)$ that depend on the imaginary time τ ($0 \leq \tau \leq \beta$), \hat{U}_σ is the many-particle propagator for a system of noninteracting fermions moving in external fields $\sigma(\tau)$, and G_σ is a Gaussian weight. To facilitate numerical evaluation the imaginary time is discretized into a finite number N_τ of points $\tau_n = n\Delta\beta$, where $\Delta\beta = \beta/N_\tau$. The calculations become exact in the limit $\Delta\beta \rightarrow 0$. We find that observables scale linearly versus $\Delta\beta$ for $\Delta\beta \leq 1/32$ and take the limit $\Delta\beta \rightarrow 0$ by a linear extrapolation.

Observables.—In AFMC, a set of configurations σ_k are sampled according to the distribution $W_\sigma = G_\sigma |\text{Tr} \hat{U}_\sigma|$ using the Metropolis algorithm [25]. Thermal expectation values of observables are then calculated from

$$\frac{\text{Tr}(\hat{\mathcal{O}} e^{-\beta\hat{H}})}{\text{Tr}(e^{-\beta\hat{H}})} \approx \frac{\sum_k \langle \hat{\mathcal{O}} \rangle_{\sigma_k} \Phi_{\sigma_k}}{\sum_k \Phi_{\sigma_k}}, \quad (2)$$

where $\langle \hat{\mathcal{O}} \rangle_\sigma = \text{Tr}(\hat{\mathcal{O}} \hat{U}_\sigma) / \text{Tr} \hat{U}_\sigma$ is the expectation of an operator $\hat{\mathcal{O}}$ at a given configuration σ_k of the auxiliary fields and $\Phi_\sigma \equiv \text{Tr}(\hat{U}_\sigma) / |\text{Tr} \hat{U}_\sigma|$ is the Monte Carlo sign.

Unlike most other AFMC calculations, we calculate the traces in (2) and in the weight function W_σ at fixed particle numbers N_\uparrow, N_\downarrow , i.e., in the canonical ensemble. This is accomplished by using an exact particle-number projection via a discrete Fourier transform [25].

Monte Carlo sign.—In general the sign Φ_σ is a sample-dependent complex phase. If the fluctuations in Φ_σ become comparable to its average value, the statistical error in (2) becomes excessively large, giving rise to the so-called Monte Carlo sign problem. However, attractive contact interactions are known to have good sign ($\Phi_\sigma = 1$ for all σ) in the grand-canonical ensemble [27], thereby

avoiding the problem. This is also the case in our canonical ensemble calculations, and can be seen as follows. The sign is determined by particle-projected two-species trace

$$\text{Tr}_{N_\uparrow, N_\downarrow} \hat{U}_\sigma = \left(\text{Tr}_{N_\uparrow} \hat{U}_\sigma^\uparrow \right) \left(\text{Tr}_{N_\downarrow} \hat{U}_\sigma^\downarrow \right), \quad (3)$$

where \hat{U}_σ^\uparrow ($\hat{U}_\sigma^\downarrow$) are the auxiliary-field propagators for spin-up (spin-down) particles. For an attractive contact interaction, \hat{U}_σ^\uparrow and $\hat{U}_\sigma^\downarrow$ are time-reversal invariant, and both particle-projected traces on the right-hand side of (3) are real. For the spin-balanced system $N_\uparrow = N_\downarrow$, we have $\text{Tr}_{N_\uparrow, N_\downarrow} \hat{U}_\sigma = (\text{Tr}_{N_\uparrow} \hat{U}_\sigma^\uparrow)^2 > 0$ so the canonical sign is also 1.

Accuracy and convergence.—The accuracy of our calculations is determined by two factors. First, the contact interaction is not an exact representation of the usual regularized delta function $V(r) = \delta(r)\partial/\partial r$ used to model cold atoms [28]. We checked its accuracy against the known analytic solution of the three-particle system and found the energy to be accurate within 1%.

Second, for the calculations to be accurate, the model space must be large enough to account for both interaction effects and thermal excitations. We have accounted for this by using model spaces that are sufficiently large for the observables of interest to be well-converged for the relevant particle number and temperatures. We demonstrate the convergence in the insets to Figs. 1(a) and 1(b); the pairing gap Δ_{gap} is well-converged by $\mathcal{N}_{\max} = 9$, and the condensate fraction n by $\mathcal{N}_{\max} = 11$. We used these values of \mathcal{N}_{\max} in our calculations, along with $\mathcal{N}_{\max} = 11$ for the heat capacity (which is also well-converged).

Algorithmic improvements.—At large β , the matrix representing the one-body propagator \hat{U}_σ becomes ill-conditioned and requires numerical stabilization. However, the computational effort for the usual stabilization method [29] increases from $\mathcal{O}(\mathcal{N}_s^3)$ to $\mathcal{O}(\mathcal{N}_s^4)$ when generalized from the grand-canonical ensemble to the canonical ensemble [30]. We have devised an improved algorithm for stabilization in the canonical ensemble which scales as $\mathcal{O}(\mathcal{N}_s^3)$ [31] and thereby makes the calculations tractable for the large model spaces necessary for convergence in this system. In particular $\mathcal{N}_{\max} = 11$ contains $\mathcal{N}_s = 364$ single-particle states and to our knowledge is the largest model space used to date for canonical-ensemble AFMC calculations.

Pairing gap.—We calculated the pairing gap Δ_{gap} by particle-number reprojection [32], in which only one Metropolis walk is needed to calculate all three energies $E(N_\uparrow - 1, N_\downarrow - 1)$, $E(N_\uparrow, N_\downarrow - 1)$ and $E(N_\uparrow, N_\downarrow)$ contributing to Δ_{gap} . We sampled the fields according to the distribution $G_\sigma |\text{Tr}_{N_\uparrow, N_\downarrow - 1} \hat{U}_\sigma|$.

Our result for the pairing gap is shown in Fig. 1(a) as a function of temperature. Here Δ_{gap} is plotted in units of $\varepsilon_F \equiv 4.0 \hbar\omega$ [33] and the temperature is given in units of $T_F \equiv \varepsilon_F/k_B$, where k_B is the Boltzmann

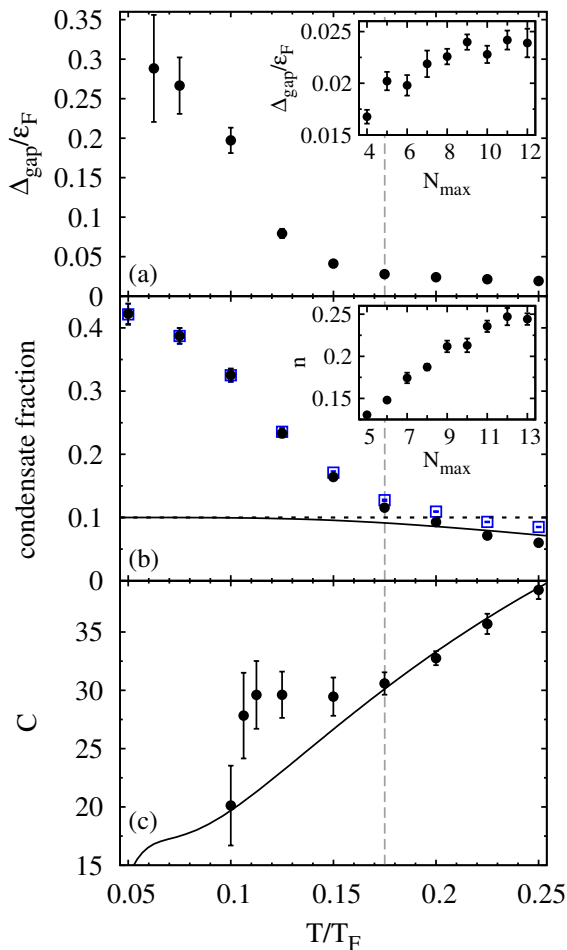


FIG. 1. Signatures of the superfluid phase transition in the trapped spin-balanced $N = 20$ atom system ($N_\uparrow = N_\downarrow = 10$). (a) AFMC results for the pairing gap Δ_{gap} vs. temperature. The inset shows the convergence of the gap as a function of the number of oscillator shells N_{max} at $T/T_F = 0.2$. (b) Condensate fraction vs. temperature. Solid circles: the scaled occupation n_0 of the $T = 0$ pair wavefunction. Open squares: the largest scaled eigenvalue n of the $L = 0$ pair correlation matrix (4). Solid line: noninteracting result. The dashed horizontal line indicates the noninteracting upper bound of $1/(N/2)$. The inset shows the convergence of n as a function of N_{max} at $T/T_F = 0.125$. (c) Heat capacity vs. temperature. The AFMC results (solid circles) are compared with the heat capacity of noninteracting fermions in the trap (solid line). The vertical dashed line in the three panels corresponds to a temperature of $T/T_F = 0.175$ (see text).

constant. At high temperature, the finite size of the system causes Δ_{gap} to remain slightly above zero. As the temperature decreases, the gap begins to depart from its high-temperature behavior at around $T/T_F \approx 0.175$; it then rises rapidly before saturating at approximately $T/T_F = 0.07$, providing a clear signature of a superfluid phase transition. We estimate the zero-temperature pairing gap by averaging the values at the lowest two temperatures, obtaining $\Delta_{\text{gap}} = 0.271(32)\varepsilon_F$. This result

is consistent with fixed-node diffusion Monte Carlo [34] and density functional theory [35] calculations.

It has been predicted that at zero temperature the energy-staggering pairing gap in a trap will be suppressed compared to its value in the homogeneous system, since in a trap unpaired particles can locate themselves in the edge of the cloud where the energy required to add an extra particle to the system is smaller [36]. More precisely, Δ_{gap} was predicted to scale at zero temperature as $\Delta_{\text{gap}} \propto (N + 1)^{1/9} \hbar \omega$. Using $\varepsilon_F = (3N)^{1/3} \hbar \omega$ [6], one therefore expects $\Delta_{\text{gap}}/\varepsilon_F \propto N^{-2/9}$ for large N . We compare this scaling with our results by computing the pairing gap at low temperature for $N = 10$ ($N_\uparrow = N_\downarrow = 5$). We find $\Delta_{\text{gap}}(5, 5) = 0.294(21)$, so that $\Delta_{\text{gap}}(10, 10)/\Delta_{\text{gap}}(5, 5) = 0.92(13)$, surprisingly close (for such small N) to the expected value of 0.866, although results at larger values of N would be required for a conclusive comparison.

Condensate fraction.—We determined the condensate fraction from the two-body density matrix. For uniform systems, there is an equivalence between off-diagonal long-range order (ODLRO) and the existence of a large eigenvalue in the two-body density matrix [37]. Thus, the existence of a large eigenvalue in this matrix is connected with the presence of superfluidity. In the trapped system, the orbital angular momentum L is conserved, and we calculate the pair correlation matrix [38]

$$C_L(ab, cd) \equiv \langle A_{LM\uparrow\downarrow}^\dagger(ab) A_{LM\uparrow\downarrow}(cd) \rangle, \quad (4)$$

where $\langle \cdot \rangle$ denotes a thermal expectation value as in Eq. (2). Here $A_{LM\uparrow\downarrow}^\dagger(ab)$ is a pair creation operator for two particles in orbitals $a = (n_a, l_a)$ and $b = (n_b, l_b)$ coupled to total angular momentum L with magnetic quantum number M , with the first particle being of the \uparrow species and the second the \downarrow species. The expectation values on the right-hand side of (4) are independent of M because of rotational invariance. Up to a $(2L + 1)$ -fold degeneracy, the eigenvalues of $C_L(ab, cd)$ are exactly those of the matrix $\langle a_{am_a\uparrow}^\dagger a_{bm_b\downarrow}^\dagger a_{dm_d\downarrow} a_{cm_c\uparrow} \rangle$, which is the orbital-space form of the density matrix studied in the uniform gas (via ODLRO) [27, 39–41]. We find that the largest eigenvalue always occurs for $L = 0$.

As the temperature decreases, the maximum eigenvalue λ_{max} becomes much larger than all others and satisfies constraints which allow for two natural definitions of a condensate fraction. The corresponding eigenvector $\varphi(ab)$ defines a pair creation operator $B^\dagger = \sum_{a,b} \varphi^*(ab) A_{00\uparrow\downarrow}^\dagger(ab)$ which satisfies $\langle B^\dagger B \rangle = \lambda_{\text{max}}$, indicating that λ_{max} is the occupation of a two-body wavefunction. For free fermions, $0 \leq \lambda_{\text{max}} \leq 1$, so no more than two fermions can occupy a paired state. However, in the presence of interactions λ_{max} can exceed 1, effectively allowing fermion pairs to “condense”. One can then show that λ_{max} sat-

isfies $0 \leq \lambda_{\max} \leq B(\mathcal{N}_s, N)$, where

$$B(\mathcal{N}_s, N) = N(\mathcal{N}_s - N/2 + 1)/2\mathcal{N}_s \leq N/2 \quad (5)$$

and \mathcal{N}_s is the number of single-particle orbitals for a single species [42]. In the limit of large \mathcal{N}_s , $B(\mathcal{N}_s, N)$ approaches $N/2$. In fact for $\mathcal{N}_{\max} = 11$ oscillator shells $\mathcal{N}_s = 364$, and $B(\mathcal{N}_s, N) = 9.75$ is quite close to $N/2 = 10$. Moreover, $\lambda_{\max} = B(\mathcal{N}_s, N)$ can be achieved for a particular many-body wavefunction (which is not necessarily an eigenstate of the system). We may therefore define a condensate fraction by $n \equiv \lambda_{\max}/(N/2)$, where $0 \leq n \leq 1$.

We can also define a condensate fraction in terms of the scaled occupation of the zero-temperature pair $B_0^\dagger \equiv B^\dagger(T=0)$, i.e., $n_0 \equiv \langle B_0^\dagger B_0 \rangle / (N/2)$. In contrast to n , n_0 measures the fraction of fully condensed pairs at finite temperature, ignoring contributions from paired particles not occupying the zero-temperature pair wavefunction. In general $n_0(T) \leq n(T)$ and equality holds in the limit $T=0$.

Fig. 1(b) shows our result for n_0 and n as a function of temperature. The two condensate fractions are nearly identical for temperatures below $T/T_F = 0.175$, while $n_0 < n$ at higher temperatures. For comparison, we plot n for a noninteracting gas (solid line) and its largest possible value of $2/N$ corresponding to $\langle B^\dagger B \rangle = 1$ (dashed line). In both cases we see a rapid increase of the condensate fraction below $T/T_F \approx 0.175$, signifying the onset of a superfluid state.

The condition $\langle B_0^\dagger B_0 \rangle > 1$ provides a definite upper bound T_{ub} in temperature for condensation to be present, since condensation requires the pair wavefunction to be occupied by more than one Fermion pair. In our system, this yields $T_{\text{ub}}/T_F \approx 0.175$, a temperature similar to the transition temperature scales for the pairing gap and the heat capacity (see below for the latter).

Pseudogap effects.—An effective way to assess pseudogap effects in this system is to compare the temperature dependence of the condensate fraction with the temperature dependence of the pairing gap. In the absence of other mitigating effects, preformed pairs of attractively interacting fermions would cause the gap to lead the condensate fraction as the temperature decreases toward T_c . Comparing Figs. 1(a) and 1(b) indicates that this does not occur: First, $\Delta_{\text{gap}}(T_{\text{ub}}) = 0.028(2)$, an insignificant fraction of its $T=0$ value. Second, below $T/T_F \approx 0.175$, the condensate fractions n and n_0 both grow simultaneously with the pairing gap Δ . Thus, we conclude that in the $N=20$ finite-size system, Δ_{gap} does not display any pseudogap effects.

Similar to our results, the t-matrix calculations of Ref. [43] for a trapped gas found a pseudogap temperature only slightly higher than the critical temperature for the unitary trapped gas. In contrast, Monte Carlo calculations for a *uniform* gas found a nonzero gap Δ

at temperatures significantly above T_c [17, 19]. In those calculations Δ was extracted from the spectral weight function (by fitting a BCS-like dispersion) rather than from energy staggering.

Note that our conclusion in the finite-size system, where the phase transition is smoothed, does not imply a pseudogap effect in Δ_{gap} will be absent for larger systems. At zero temperature, fixed-node quantum Monte Carlo and density-functional calculations predict that finite-size effects become negligible for more than 50 particles [44], while lattice Monte Carlo computations have found that shell effects still persist at the 2% level above 40 particles [45]. It would be interesting to use our method to study the finite-temperature behavior of the system as a function of N .

Heat capacity.—Fig. 1(c) shows our results for the heat capacity $C = dE/dT$ as a function of temperature. We calculated C by numerically differentiating the energy inside the path integral; this method takes into account correlated errors and greatly reduces the statistical error compared to differentiation after calculating $E(T)$ [46]. At high temperatures, the heat capacity agrees with that of a noninteracting trapped Fermi gas (solid line). As the temperature decreases below $T/T_F = 0.175$, it begins to deviate from its non-interacting limit, remaining elevated until dropping rapidly at around $T/T_F = 0.11$ —a smoothed but obvious signature of the lambda peak observed recently in the thermodynamic limit [12]. The temperature at which this structure emerges, $T/T_F \approx 0.175$, is commensurate with the rise of the pairing gap and the temperature at which the condensate fraction n exceeds its noninteracting limit.

In conclusion, we have calculated the energy staggering pairing gap, condensate fraction, and heat capacity for an unpolarized system of $N=20$ trapped cold atoms at unitarity using a quantum Monte Carlo method. Clear signatures of the superfluid phase transition exist in each of these quantities. In this finite-size trapped system, the gap does not lead the condensate fraction as temperature decreases and thus provides no clear signature of a pseudogap phase. The same method can be applied on either side of the BEC-BCS crossover, and could potentially be used to study finite-size scaling.

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